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Radiative efficiency estimation of organic substance based on group contribution method

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Abstract

The development of organic working fluid has entered the environment protection era. Ozone depletion potential (ODP) and global warming potential (GWP) are two most important indices of the organic working fluid. Nowadays, more and more attention has been paid to GWP. The calculation of GWP is an extremely complicated process which involves interactions between surface and atmosphere such as atmospheric radiative transfer and atmospheric chemical reactions. GWP of a substance is related to its atmospheric abundance and is a variable in itself. However, radiative efficiency is an intermediate parameter for GWP calculation and it is a constant value used to describe inherent property of a substance. In this paper, the group contribution method was adopted to estimate the radiative efficiency of the organic substance which contains more than one carbon atom. In most cases, the estimation value and the standard value are in a good agreement and most errors are less than 20%, and the biggest estimation error occurs in the estimation of the radiative efficiency of fluorinated ethers which contains several carbon atoms because of the complicated structure of fluorinated ethers compared with hydrocarbon. This estimation method can be used to predict the radiative efficiency of newly developed organic working fluids and its accuracy can meet the requirement of engineering application.

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Keywords: Organic substance; Global warming potential; Radiative efficiency; Group contribution method

1. Introduction

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In thermodynamics, there are mainly two applications of organic working fluid. One is used as refrigerant in refrigeration cycle which is the primary application of the organic working fluid. The other is low-grade heat recovery through an organic Rankine cycle(ORC). Indicators for quantitative comparison of the various organic working fluids are ODP(Ozone depletion Potential) and GWP, which are closely related to their atmospheric lifetime(ALT). ODP of one- and two-carbon HFCs(hydrofluorocarbons) and HCFCs((hydrochlorofluorocarbons) can already be estimated with a good precision[1]. However, GWP of organic working fluid cannot be estimated due to its extreme calculation complication. The calculation of GWP involves interactions between surface and atmosphere such as atmospheric radiative transfer and atmospheric chemical reactions. From the definition of GWP given by Intergovernmental Panel on Climate Change(IPCC)[2], it can be seen that GWP of a substance is related to its atmospheric abundance and is a variable in itself. However, radiative efficiency is an intermediate parameter for GWP calculation and it is a constant value used to describe inherent property of a substance. The group contribution method has been widely used and achieved good results in property estimation of organic matter due to its simplicity, reliable accuracy, and wide applicability[3-5]. Therefore, in this paper, the group contribution method was adopted to estimate the radiative efficiency of the organic substance which contains more than one carbon atom. The estimation result offers a good and convenient reference for the development of new organic working fluids.

2. Group Division

Molecule was made up of atoms through chemical bond. The existence of intermolecular force makes the distribution of atoms in space not random and homogeneous. The distribution shows a group characteristic via some certain space structures. These groups have an important influence to many properties of substance and this influence remains the same in difference substance. The molecular property is an additive property. The element contribution remains the same in different molecule. In this paper, the group is divided according to the radiative efficiency published by IPCC[2] and the different type of substance. Considering the newly developed organic working fluid usually contains more than one carbon atom, only radiative efficiency of organic matters which contain 2 to 4 carbon atoms are calculated. Table 1 lists the groups and their contribution to the organic matters of different types.

Table 1. Groups and their contribution to the organic matters of different types

Number	Group	Contribution to radiative efficiency of CFC, HCFC, and Halon	Contribution to radiative efficiency of HFC	Contribution to radiative efficiency of fluorinated ethers
1	$-CH_3$	0.005	0.015	0.005
2	$-CCl_3$	0.015	/	/
3	$-CF_3$	0.025	0.115	0.115
4	$-CF_2-$	0.06	0.03	0.01
5	$-CClF_2$	0.155	/	/
6	$-CCl_2F$	0.145	/	/
7	$-CBrF_2$	0.165	/	/
8	$-CHCl_2$	0.115	/	/
9	-CHClF	0.195	/	/
10	$-CH_2-$	/	0.05	0.002
11	$-CHF_2$	/	0.095	0.095
12	$-CH_2F$	/	0.145	/
13	-CHF-	/	0.03	/
14	-CHCl-	/	/	0.002
15	-O-	/	/	0.23

NOTE: the unit in table is $W \cdot m^{-2} \cdot ppb^{-1}$

3. Result and Discussion

Table 2 lists the estimation results of radiative efficiency of CFC, HCFC, and Halon. Relative error between estimation results and standard value published by IPCC can also be found in Table 2. Table 3 lists the estimation results and relative error of HFC and the corresponding value of fluorinated ethers can be found in Table 4.From these tables, it can be seen that in most cases, the estimation value and the standard value are in a good agreement and most errors are less than 20%, and the biggest estimation error occurs in the estimation of the radiative efficiency of fluorinated ethers which contains several carbon atoms because of the complicated structure of fluorinated ethers compared with hydrocarbon. The estimation accuracy is as fine as that of similar work on estimation of tropospheric lifetimes and ozone-depletion potentials of one- and two-carbon HFC and HCFC by other researchers[1].

Table 2. Estimation results and relative error of CFC, HCFC, and Halon

Working fluid	Chemical formula	Combination of the group(in number)	Standard value of IPCC/ $W\cdot m^{-2}\cdot ppb^{-1}$	Estimation Result/ $W\cdot m^{-2}\cdot ppb^{-1}$	Relative Error/%
CFC-113	CCl_2FCClF_2	5+6	0.3	0.3	0
CFC-114	$CClF_2CClF_2$	5+5	0.31	0.31	0
CFC-115	$CClF_2CF_3$	3+5	0.18	0.18	0
Halon-2402	$CBrF_2CBrF_2$	7+7	0.33	0.33	0
Methyl chloroform	CH_3CCl_3	1+2	0.06	0.02	66.67
HCFC-123	$CHCl_2CF_3$	3+8	0.14	0.14	0
HCFC-124	$CHClFCF_3$	3+9	0.22	0.22	0
HCFC-141b	CH_3CCl_2F	1+6	0.14	0.15	7.14
HCFC-142b	CH_3CClF_2	1+5	0.2	0.16	20
HCFC-225ca	$CHCl_2CF_2CF_3$	3+4+8	0.2	0.2	0
HCFC-225cb	$CHClFCF_2CClF_2$	4+5+9	0.32	0.41	28.13

Table 3. Estimation results and relative error of HFC

Working fluid	Chemical formula	Combination of the group(in number)	Standard value of IPCC/ $W\cdot m^{-2}\cdot ppb^{-1}$	Estimation Result/ $W\cdot m^{-2}\cdot ppb^{-1}$	Relative Error/%
HFC-125	CHF_2CF_3	3+11	0.23	0.21	8.70
HFC-134a	CH_2FCF_3	3+12	0.16	0.26	62.5
HFC-143a	CH_3CF_3	1+3	0.13	0.13	0
HFC-152a	CH_3CHF_2	1+11	0.09	0.11	22.22
HFC-227ea	CF_3CHFCF_3	3+3+13	0.26	0.26	0
HFC-236fa	$CF_3CH_2CF_3$	3+3+10	0.28	0.28	0
HFC-245fa	$CHF_2CH_2CF_3$	3+10+11	0.28	0.26	7.14
HFC-365mfc	$CH_3CF_2CH_2CF_3$	1+3+4+10	0.21	0.21	0

Table 4. Estimation results and relative error of fluorinated ethers

Working fluid	Chemical formula	Combination of the group(in number)	Standard value of IPCC/ $W\cdot m^{-2}\cdot ppb^{-1}$	Estimation Result/ $W\cdot m^{-2}\cdot ppb^{-1}$	Relative Error/%
HFE-125	CHF_2OCF_3	3+11+15	0.44	0.44	0
HFE-134	CHF_2OCHF_2	11+11+15	0.45	0.42	6.67
HFE-143a	CH_3OCF_3	1+3+15	0.27	0.35	29.63
HCFE-235da2	$CHF_2OCHClCF_3$	3+11+14+15	0.38	0.442	16.32
HFE-245cb2	$CH_3OCF_2CHF_2$	1+4+11+15	0.32	0.34	6.25
HFE-245fa2	$CHF_2OCH_2CF_3$	3+10+11+15	0.31	0.442	42.58
HFE-254cb2	$CH_3OCF_2CHF_2$	1+4+11+15	0.28	0.34	21.43
HFE-347mcc3	$CH_3OCF_2CF_2CF_3$	1+3+4+4+15	0.34	0.37	8.82
HFE-347pcf2	$CHF_2CF_2OCH_2CF_3$	3+4+10+11+15	0.25	0.452	80.8
HFE-356pcc3	$CH_3OCF_2CF_2CHF_2$	1+4+4+11+15	0.93	0.35	62.37

4. Conclusion

The group contribution method was adopted to estimate the radiative efficiency of the organic substance which contains more than one carbon atom. In most cases, the estimation value and the standard value are in a good agreement and most errors are less than 20%, and the biggest estimation error occurs in the estimation of the radiative efficiency of fluorinated ethers which contains several carbon atoms because of the complicated structure of fluorinated ethers compared with hydrocarbon. This estimation method can be used to predict the radiative efficiency of newly developed organic working fluids and its accuracy can meet the requirement of engineering application.

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Biography

Dr. Xinxin Zhang graduated from Xi'an Jiaotong University and was a joint training doctoral student of Nagoya University supported by China Scholarship Council. Now he works in Beijing University of Technology and his research interest is new-type and combined thermodynamic cycle and waste heat recovery through thermodynamic approach.